Cartesian coordinates of theoretically optimized geometries:

1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.765499	1.016412
2	6	0	0.000000	3.033030	1.533201
3	6	0	0.000000	1.736787	-0.349943
4	6	0	0.000000	2.864195	-1.175852
5	6	0	0.000000	4.162325	-0.627955
6	6	0	0.000000	4.206481	0.780335
7	7	0	0.000000	-1.765499	1.016412
8	44	0	0.000000	0.000000	2.445231
9	6	0	0.000000	-3.033030	1.533201
10	6	0	0.000000	-4.206481	0.780335
11	6	0	0.000000	-4.162325	-0.627955
12	6	0	0.000000	-2.864195	-1.175852
13	6	0	0.000000	-1.736787	-0.349943
14	6	0	0.000000	-5.395563	-1.463284
15	6	0	0.000000	-5.339935	-2.875824
16	6	0	0.000000	-6.504889	-3.633237
17	7	0	0.000000	-7.730313	-3.036736
18	6	0	0.000000	-7.824619	-1.679789
19	6	0	0.000000	-6.682832	-0.883363
20	6	0	0.000000	-8.958867	-3.888997
21	6	0	0.000000	5.395563	-1.463284
22	6	0	0.000000	6.682832	-0.883363
23	6	0	0.000000	7.824619	-1.679789
24	7	0	0.000000	7.730313	-3.036736
25	6	0	0.000000	6.504889	-3.633237
26	6	0	0.000000	5.339935	-2.875824
27	6	0	0.000000	8.958867	-3.888997
28	7	0	2.167514	0.000000	2.388475
29	7	0	0.000000	-1.357355	4.180155
30	7	0	0.000000	1.357355	4.180155
31	7	0	-2.167514	0.000000	2.388475
32	1	0	0.000000	3.146861	2.601268
33	1	0	0.000000	2.691207	-2.245341
34	1	0	0.000000	5.140566	1.328655
35	1	0	0.000000	-3.146861	2.601268
36	1	0	0.000000	-5.140566	1.328655
37	1	0	0.000000	-2.691207	-2.245341
38	1	0	0.000000	-4.404012	-3.418909
39	1	0	0.000000	-6.488411	-4.716396
40	1	0	0.000000	-8.819960	-1.253636
41	1	0	0.000000	-6.838483	0.187281
42	1	0	0.895319	-8.965107	-4.514417
43	1	0	0.000000	-9.843314	-3.252659
44	1	0	-0.895319	-8.965107	-4.514417
45	1	0	0.000000	6.838483	0.187281
46	1	0	0.000000	8.819960	-1.253636
47	1	0	0.000000	6.488411	-4.716396
48	1	0	0.000000	4.404012	-3.418909
49	1	0	0.000000	9.843314	-3.252659
50	1	0	0.895319	8.965107	-4.514417
51	1	0	-0.895319	8.965107	-4.514417
52	1	0	2.592591	0.826947	2.817732

53	1	0	2.592591	-0.826947	2.817732
54	1	0	0.824987	-1.171100	4.760229
55	1	0	-0.824987	-1.171100	4.760229
56	1	0	0.824987	1.171100	4.760229
57	1	0	0.000000	2.364984	4.016819
58	1	0	-2.592591	0.826947	2.817732
59	1	0	-2.442467	0.000000	1.402410
60	1	0	-2.592591	-0.826947	2.817732
61	1	0	-0.824987	1.171100	4.760229
62	1	0	2.442467	0.000000	1.402410
63	1	0	0.000000	-2.364984	4.016819
64	1	0	0.000000	0.772490	-0.821543
65	1	0	0.000000	-0.772490	-0.821543

1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.599117	1.062232
2	6	0	-1.152713	2.180604	0.612450
3	6	0	1.152713	2.180604	0.612450
4	6	0	1.191443	3.301036	-0.218486
5	6	0	0.000000	3.916585	-0.657858
6	6	0	-1.191443	3.301036	-0.218486
7	7	0	0.000000	-1.599117	1.062232
8	44	0	0.000000	0.000000	2.500586
9	6	0	-1.152713	-2.180604	0.612450
10	6	0	-1.191443	-3.301036	-0.218486
11	6	0	0.000000	-3.916585	-0.657858
12	6	0	1.191443	-3.301036	-0.218486
13	6	0	1.152713	-2.180604	0.612450
14	6	0	0.000000	-5.137119	-1.511735
15	6	0	1.201290	-5.751628	-1.931668
16	6	0	1.178620	-6.903794	-2.710129
17	7	0	0.000000	-7.470246	-3.089923
18	6	0	-1.178620	-6.903794	-2.710129
19	6	0	-1.201290	-5.751628	-1.931668
20	6	0	0.000000	-8.695466	-3.946782
21	6	0	0.000000	5.137119	-1.511735
22	6	0	-1.201290	5.751628	-1.931668
23	6	0	-1.178620	6.903794	-2.710129
24	7	0	0.000000	7.470246	-3.089923
25	6	0	1.178620	6.903794	-2.710129
26	6	0	1.201290	5.751628	-1.931668
27	6	0	0.000000	8.695466	-3.946782
28	7	0	2.183903	0.000000	2.649667
29	7	0	0.000000	-1.538237	4.043945
30	7	0	0.000000	1.538237	4.043945
31	7	0	-2.183903	0.000000	2.649667
32	1	0	-2.087991	1.744234	0.929441
33	1	0	2.168934	3.674266	-0.498920
34	1	0	-2.168934	3.674266	-0.498920
35	1	0	-2.087991	-1.744234	0.929441
36	1	0	-2.168934	-3.674266	-0.498920
37	1	0	2.168934	-3.674266	-0.498920
38	1	0	2.175795	-5.363865	-1.665846
39	1	0	2.087667	-7.391419	-3.039987
40	1	0	-2.087667	-7.391419	-3.039987

41	1	0	-2.175795	-5.363865	-1.665846
42	1	0	0.887186	-9.290792	-3.728782
43	1	0	-0.887186	-9.290792	-3.728782
44	1	0	0.000000	-8.400807	-4.999247
45	1	0	-2.175795	5.363865	-1.665846
46	1	0	-2.087667	7.391419	-3.039987
47	1	0	2.087667	7.391419	-3.039987
48	1	0	2.175795	5.363865	-1.665846
49	1	0	-0.887186	9.290792	-3.728782
50	1	0	0.887186	9.290792	-3.728782
51	1	0	0.000000	8.400807	-4.999247
52	1	0	2.514376	0.823033	3.164235
53	1	0	2.514376	-0.823033	3.164235
54	1	0	0.817895	-1.492783	4.660349
55	1	0	-0.817895	-1.492783	4.660349
56	1	0	0.817895	1.492783	4.660349
57	1	0	0.000000	2.465209	3.606091
58	1	0	-2.514376	0.823033	3.164235
59	1	0	-2.671468	0.000000	1.750070
60	1	0	-2.514376	-0.823033	3.164235
61	1	0	-0.817895	1.492783	4.660349
62	1	0	2.671468	0.000000	1.750070
63	1	0	0.000000	-2.465209	3.606091
64	1	0	2.087991	1.744234	0.929441
65	1	0	2.087991	-1.744234	0.929441

1c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.539722	1.125512	-0.090464
2	6	0	-1.581276	0.028474	0.727770
3	6	0	-2.620032	1.305923	-0.913785
4	6	0	-3.732415	0.464012	-0.921470
5	6	0	-3.792786	-0.642071	-0.047608
6	6	0	-2.667364	-0.848595	0.779072
7	7	0	1.539685	1.125389	0.089850
8	44	0	0.000009	2.550068	-0.000344
9	6	0	2.619768	1.306878	0.913280
10	6	0	3.732064	0.464947	0.922473
11	6	0	3.792639	-0.642486	0.050303
12	6	0	2.667576	-0.850002	-0.776577
13	6	0	1.581502	0.027250	-0.726874
14	6	0	4.984991	-1.527855	0.000033
15	6	0	5.392428	-2.145512	-1.202013
16	6	0	6.524418	-2.953322	-1.229819
17	7	0	7.259894	-3.167548	-0.102498
18	6	0	6.891895	-2.591106	1.074914
19	6	0	5.767263	-1.773712	1.149612
20	6	0	8.489962	-4.015570	-0.176925
21	6	0	-4.985047	-1.527447	0.000187
22	6	0	-5.392044	-2.141560	1.207033
23	6	0	-6.525912	-2.949958	1.237677
24	7	0	-7.260352	-3.166077	0.112251
25	6	0	-6.891718	-2.591517	-1.067927
26	6	0	-5.768522	-1.775700	-1.145334
27	6	0	-8.488531	-4.019002	0.156793
28	7	0	0.188815	2.552312	-2.161991

29	7	0	1.515071	4.127878	0.062850
30	7	0	-1.514639	4.127977	-0.067246
31	7	0	-0.188604	2.555055	2.159349
32	1	0	-0.711167	-0.144977	1.349386
33	1	0	-4.555406	0.707473	-1.584989
34	1	0	-2.610426	-1.697964	1.451660
35	1	0	2.595017	2.166596	1.572482
36	1	0	4.554951	0.709318	1.585783
37	1	0	2.610752	-1.700182	-1.448150
38	1	0	4.861981	-1.988235	-2.133621
39	1	0	6.870133	-3.430475	-2.138827
40	1	0	7.508707	-2.799799	1.940187
41	1	0	5.508640	-1.361530	2.117691
42	1	0	9.305822	-3.430761	-0.608925
43	1	0	8.766062	-4.345058	0.824609
44	1	0	8.289863	-4.891199	-0.796295
45	1	0	-4.862109	-1.982018	2.138507
46	1	0	-6.868719	-3.423817	2.148956
47	1	0	-7.510990	-2.804477	-1.930985
48	1	0	-5.510005	-1.364826	-2.114037
49	1	0	-8.546309	-4.524429	1.120402
50	1	0	-9.370939	-3.388842	0.023123
51	1	0	-8.438736	-4.766852	-0.636770
52	1	0	0.050370	3.472532	-2.592006
53	1	0	1.126984	2.237039	-2.428432
54	1	0	1.269419	4.908580	-0.554368
55	1	0	1.659254	4.527527	0.995729
56	1	0	-1.659402	4.526078	-1.000697
57	1	0	-2.421435	3.772338	0.251973
58	1	0	-1.127060	2.240975	2.426196
59	1	0	0.481060	1.913079	2.594956
60	1	0	-0.049293	3.475654	2.588279
61	1	0	-1.268408	4.909667	0.548483
62	1	0	-0.481458	1.910439	-2.596807
63	1	0	2.422020	3.771533	-0.255148
64	1	0	-2.595399	2.164729	-1.574178
65	1	0	0.711646	-0.146995	-1.348627

12 (C_{2v})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.296630	1.642266
2	6	0	0.000000	2.654809	1.723707
3	6	0	0.000000	0.737829	0.377572
4	6	0	0.000000	1.541937	-0.774617
5	6	0	0.000000	2.950982	-0.690710
6	6	0	0.000000	3.491797	0.613990
7	7	0	0.000000	-1.296630	1.642266
8	44	0	0.000000	0.000000	3.240963
9	6	0	0.000000	-2.654809	1.723707
10	6	0	0.000000	-3.491797	0.613990
11	6	0	0.000000	-2.950982	-0.690710
12	6	0	0.000000	-1.541937	-0.774617
13	6	0	0.000000	-0.737829	0.377572
14	6	0	0.000000	-3.839798	-1.887635
15	6	0	0.000000	-3.335191	-3.208788
16	6	0	0.000000	-4.193519	-4.301421
17	7	0	0.000000	-5.546031	-4.133979

18	6	0	0.000000	-6.071216	-2.879602
19	6	0	0.000000	-5.246699	-1.758202
20	6	0	0.000000	-6.435312	-5.336573
21	6	0	0.000000	3.839798	-1.887635
22	6	0	0.000000	5.246699	-1.758202
23	6	0	0.000000	6.071216	-2.879602
24	7	0	0.000000	5.546031	-4.133979
25	6	0	0.000000	4.193519	-4.301421
26	6	0	0.000000	3.335191	-3.208788
27	6	0	0.000000	6.435312	-5.336573
28	7	0	2.167698	0.000000	3.249025
29	7	0	0.000000	-1.449652	4.898183
30	7	0	0.000000	1.449652	4.898183
31	7	0	-2.167698	0.000000	3.249025
32	1	0	0.000000	3.090537	2.712596
33	1	0	0.000000	1.054084	-1.741588
34	1	0	0.000000	4.558113	0.798683
35	1	0	0.000000	-3.090537	2.712596
36	1	0	0.000000	-4.558113	0.798683
37	1	0	0.000000	-1.054084	-1.741588
38	1	0	0.000000	-2.274514	-3.422477
39	1	0	0.000000	-3.829930	-5.321748
40	1	0	0.000000	-7.150789	-2.794657
41	1	0	0.000000	-5.744239	-0.798072
42	1	0	0.895780	-6.240955	-5.930380
43	1	0	0.000000	-7.477426	-5.018574
44	1	0	-0.895780	-6.240955	-5.930380
45	1	0	0.000000	5.744239	-0.798072
46	1	0	0.000000	7.150789	-2.794657
47	1	0	0.000000	3.829930	-5.321748
48	1	0	0.000000	2.274514	-3.422477
49	1	0	0.000000	7.477426	-5.018574
50	1	0	0.895780	6.240955	-5.930380
51	1	0	-0.895780	6.240955	-5.930380
52	1	0	2.568993	0.826494	3.702483
53	1	0	2.568993	-0.826494	3.702483
54	1	0	0.821038	-1.332297	5.501926
55	1	0	-0.821038	-1.332297	5.501926
56	1	0	0.821038	1.332297	5.501926
57	1	0	0.000000	2.428965	4.600751
58	1	0	-2.568993	0.826494	3.702483
59	1	0	-2.502240	0.000000	2.281052
60	1	0	-2.568993	-0.826494	3.702483
61	1	0	-0.821038	1.332297	5.501926
62	1	0	2.502240	0.000000	2.281052
63	1	0	0.000000	-2.428965	4.600751

12 (C_1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.300470	-1.620217	0.048422
2	6	0	-2.659259	-1.706769	0.100253
3	6	0	-0.736872	-0.358055	0.010040
4	6	0	-1.538259	0.796279	-0.011018
5	6	0	-2.943397	0.702015	0.033435
6	6	0	-3.496496	-0.594094	0.101511

7	7	0	1.300446	-1.620225	-0.048698
8	44	0	-0.000017	-3.213304	0.000026
9	6	0	2.659226	-1.706790	-0.100744
10	6	0	3.496476	-0.594125	-0.101997
11	6	0	2.943396	0.701981	-0.033685
12	6	0	1.538265	0.796261	0.010929
13	6	0	0.736862	-0.358062	-0.010177
14	6	0	3.835102	1.891383	0.001809
15	6	0	3.556708	3.010465	0.813351
16	6	0	4.443568	4.084482	0.859777
17	7	0	5.587489	4.079400	0.122092
18	6	0	5.880326	3.017764	-0.681736
19	6	0	5.027174	1.922263	-0.756099
20	6	0	6.548922	5.223875	0.195779
21	6	0	-3.835085	1.891431	-0.001978
22	6	0	-5.027326	1.922128	0.755688
23	6	0	-5.880476	3.017618	0.681376
24	7	0	-5.587481	4.079447	-0.122151
25	6	0	-4.443406	4.084719	-0.859580
26	6	0	-3.556536	3.010695	-0.813206
27	6	0	-6.548709	5.224134	-0.195205
28	7	0	0.089712	-3.247925	2.164401
29	7	0	1.504163	-4.816521	-0.054899
30	7	0	-1.504210	-4.816471	0.055767
31	7	0	-0.089769	-3.248893	-2.164333
32	1	0	-3.087471	-2.699538	0.134580
33	1	0	-1.066813	1.772493	-0.040299
34	1	0	-4.569270	-0.752170	0.117659
35	1	0	3.087411	-2.699564	-0.135267
36	1	0	4.569247	-0.752202	-0.118331
37	1	0	1.066837	1.772479	0.040352
38	1	0	2.680405	3.050653	1.449567
39	1	0	4.268075	4.947897	1.489172
40	1	0	6.800322	3.072695	-1.251529
41	1	0	5.299506	1.114482	-1.425249
42	1	0	7.468042	4.891725	0.684079
43	1	0	6.768305	5.577829	-0.813377
44	1	0	6.106155	6.035848	0.771948
45	1	0	-5.299802	1.114182	1.424581
46	1	0	-6.800592	3.072437	1.250991
47	1	0	-4.267775	4.948284	-1.488726
48	1	0	-2.680120	3.051028	-1.449255
49	1	0	-6.763103	5.581653	0.813789
50	1	0	-6.108369	6.033843	-0.776387
51	1	0	-7.470293	4.890799	-0.677991
52	1	0	0.116700	-4.194778	2.555946
53	1	0	0.923535	-2.755805	2.499586
54	1	0	2.173714	-4.729840	0.715986
55	1	0	1.099280	-5.755732	0.022997
56	1	0	-1.099321	-5.755734	-0.021458
57	1	0	-2.042275	-4.806538	0.928025
58	1	0	-0.923706	-2.757116	-2.499742
59	1	0	0.723796	-2.774630	-2.567704
60	1	0	-0.116558	-4.195935	-2.555436
61	1	0	-2.173654	-4.730294	-0.715266
62	1	0	-0.723970	-2.773648	2.567520
63	1	0	2.042116	-4.807175	-0.927234

Complete Reference 25:

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